Internship title: Defect recognition in coherent diffraction patterns

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The CEA (cea.fr) is a major French research agency and IRIG (Irig) is one of its institutes, devoted to fundamental research, in the Grenoble Minatec (Minatec.org) area. The ESRF (European Synchrotron Radiation Facility, esrf.eu) is a multinational research institute, situated in Grenoble, France. It operates one of the most powerful synchrotron x-ray sources. Both institutes offer a highly dynamic, exciting and multinational working environment in the French Alps.

Context

Identifying defects in nanomaterials is a challenge. Defects can dramatically influence the (mechanical, electrical, magnetic, optical, chemical, *etc*) properties of materials. Coherent x-ray diffraction is a powerful emerging technique to probe the structure of nanomaterials in a non-destructive way and in three-dimensions (3D). Crystal defects in nanostructures induce strong distortions in diffraction patterns and their identification based on their signatures on diffraction patterns is not straightforward [1]. The availabilities of new 2D-detectors and fast computation are now opening a new area of research in quantitative coherent x-ray diffraction: determining the 3D structure of the measured nano-object.

Goals

This internship is focused on the development of an algorithm based on neural network to recognize and identify defect signatures in coherent diffraction patterns.
The student will first be introduced to the basics of coherent diffraction, and atomistic simulations applied to the study of structural defects in nanomaterials. Initially, we will provide him/her datasets of a catalog of defects inside nanostructures obtained using atomistic simulations. Subsequently, he/she will use atomistic simulations in order to expand the dataset and try for instance to capture the influence of the defect type or position. The diffraction patterns will be calculated in the kinematical approximation using the PyNX code [2]. The simulated datasets will be used to train and evaluate the machine learning model based on neural network first in 2D and ultimately in 3D. The student will then evaluate the algorithm with real datasets collected at The European synchrotron (ESRF) and provide analysis on performance improvements. **The development and optimization of this network on simulated and real datasets are the major goals of the internship.** Identifying defects in coherent diffraction patterns will allow to improve performances of nanomaterials *via* defect engineering which has many applications in the field of material science [3,4].
The ESRF has recently upgraded and will be commissioning during the internship. This is a unique opportunity to be a part of the most Brilliant synchrotron light source in the world. Coherent diffraction imaging will benefit to the tune of a factor of 30 increased coherent flux so there will be plenty of opportunities to make a strong impact.

Prerequisites

The applicant will be either in the first or second year of a Master or Engineer school related to computing sciences. We expect the candidate to have broad interests and an excellent knowledge of computer science, machine learning, artificial intelligence and analysis as well as a strong background in physics and mathematics (linear algebra, numeric methods, statistics). Knowledge and interest in material science and crystallography are a plus. The applicant should have very good skills in programming (Python). He/she should have good interpersonal, communication, organisational and presentational skills. The working language is English.

[1] M. Dupraz, G. Beutier, D. Rodney, D. Mordehai, and M. Verdier, J. Appl. Cryst. **48**, 621 (2015).
[2] O. Mandula, M. Elzo Aizarna, J. Eymery, M. Burghammer, and V. Favre-Nicolin, J. Appl. Cryst. **49**, 1842 (2016).
[3] B.T. Sneed *et al.*, Nanoscale **7**, 12248 (2015).
[4] X. Wu *et al.*, Sci. Rep **5**, 11728(2015).